

Computer Analysis of the Field Ion Images of Platinum Irradiated with Ar^+ ($E = 30$ keV) Ions

V A Ivchenko^{1,2} and V V Ovchinnikov^{1,2}

¹Institute of Electrophysics, Ural Branch of Russian Academy of Sciences,
Amundsena street 106, Yekaterinburg, 620016, Russia

²Ural Federal Technical University named after the First President of Russia B.N.
Yeltsin, Mira street 19, Yekaterinburg, 620002, Russia

E-mail: viae05@rambler.ru

Abstract. The work presents the field ion microscopy images of the surface atomic layers of irradiated platinum (layer-by-layer from 1st to 5th and more distant). A specially developed algorithm and software were used for image analysis to study the effect of Ar^+ ions ($E = 30$ keV) on the subsurface atomic structure of pure platinum. The coordinates of atoms, the brightness of their images, and their sizes were determined. The curves of the distribution of the brightness and atomic radii were built. It is shown that the width of the distributions significantly decreases when moving from the damaged surface deep into the platinum bulk, whereas the number of atoms in the field ion microscopy images increases. Field ion microscopy images with only those atoms whose brightness (or radius) is in certain range were synthesized (these atoms can be highlighted in the ionic field microscopy images). It has been established that damaged zones include the images of atoms with both abnormally low and abnormally high radii. The principal possibility of reconstruction of the 3D-picture of the irradiated metal at a temperature of liquid nitrogen ($T \sim 77$ K) is shown.

1. Introduction

A problem of paramount importance in the radiation physics of solids is a detailed study of the effect of different types of ionizing radiation on structural-phase state of irradiated media. The topical problems in developing the methods of modification of structure and properties of materials by the beams of accelerated ions are related to the depth of occurring structural changes and phase transformations as well as to defining the types of the radiation-induced defects and the peculiarities of their distribution in the bulk of material. In case of cascade-forming irradiation, the interest lies in experimental study of the structure of the atomic displacement cascades passage zones, the so-called “depleted zones” [1-3], containing different types of surviving defects after the stages of thermal spikes and intra-cascade diffusion.

Field ion microscopy (FIM) is an in-situ experimental method allowing the nature of radiation-induced lattice damage to be studied at an atomic level. Just as importantly, the method, along with visualization of an atomic-pure surface of irradiated materials, also allows the controlled removal of surface atoms under an electric field at cryogenic temperatures.

Field ion micropictures include images of thousands of atoms located at both the regular lattice sites and in the areas containing different types of defects. The source data for quantitative analysis of a lattice state would be the data on coordinates, brightness, dimensions, as well as features of surface



atom image shapes, depending on the depth of location of layers under exposure to different external factors.

As a result, a series of dependences may be derived. A promising method in analyzing defect structure and atoms dynamics is reconstruction of the imaged atomic size and brightness distribution functions for subsurface and more remote layers. The most important fundamental task is digital reconstruction of a 3D structure.

This paper presents the results of analysis of field ion images of pure platinum surface atomic layers after irradiation with Ar^+ ($E = 30$ keV) ions with application of an algorithm and a computer software developed specifically for this purpose on the basis of the mathematical pattern recognition techniques.

2. Experimental

The object under investigation was 99.99% pure polycrystalline platinum. The specimens for exposure to irradiation and subsequent studying using a field ion microscope were needles (with 30-50 nm tip point radius of curvature) made from wire blanks by the method of electrochemical polishing. Irradiation of a needle-shaped platinum emitter preliminarily certified under a field ion microscope was carried out with singly-charged accelerated (to $E = 30$ keV) Ar^+ ions to a fluence of $F = 10^{16}$ ion/cm², at 150 $\mu\text{A}/\text{cm}^2$ ion current density ($T = 70^\circ\text{C}$ at needle basis).

The irradiated specimen tip was again placed under a microscope and, by registration with a photo or video camera of surface field ion micropictures at controlled removal of surface atoms, experimental data were collected for further analysis of the subsurface volume. The surface micropictures were registered so as to allow a minimum number of evaporated atoms in the intervals between shots. In this paper the intervals between the first five micropictures were the times of evaporation under an electric field of one atomic layer (001). Such procedure is necessary for precision study of lattice defects appearing under the action of accelerated Ar^+ ions.

The field ion microscope was outfitted with a microchannel ion-electron converter enhancing 10^4 times the brightness of ion images. Liquid nitrogen served as a coolant ($T = 77$ K), and spectrally pure neon was used as an imaging gas.

3. Results and discussions

Figure 1a shows an ionic micropicture taken of a platinum specimen certified prior to the irradiation. After exposure of the metal to an argon-ion beam, Figure 1b, an ionic contrast was registered which is not typical for an ionic micropicture of a defect-free metal. Micropictures of platinum surface irradiated with 30-keV argon ions to fluence $F = 10^{16}$ cm⁻² (ion/cm²) display breaks of a (regular before irradiation) circular pattern of ionic contrast. These are the irregularities in the contrast circular pattern that are interpreted as crystal structure defects. The defect type is identified in the course of the controlled removal of surface atoms under an electric field.

In the course of surface atoms removal, a fairly large number of microphotographs of the irradiated metal surface were obtained (each layer from 1st to 88th), sufficient for detailed description of the subsurface volume.

The algorithm of identifying single atoms and fixing their coordinates is based on application of the maximum of brightness function $Y(x, y)$ criteria (where x and y are image coordinates). The first-order

$\frac{\partial Y}{\partial x}, \frac{\partial Y}{\partial y}$, also the second-order $\frac{\partial^2 Y}{\partial x^2}, \frac{\partial^2 Y}{\partial y^2}$, derivatives were analyzed in finite difference

representations with account for the discrete nature of digital images.

Atomic image coordinates, brightness, dimensions were determined and atomic brightness and radii values distribution functions were designed with the use of computer software. After that the field ion images of all atoms, or only of the atoms with the brightness or radii lying within the preset limits, were synthesized (colour marking of different groups of atoms in the ion field images is feasible).

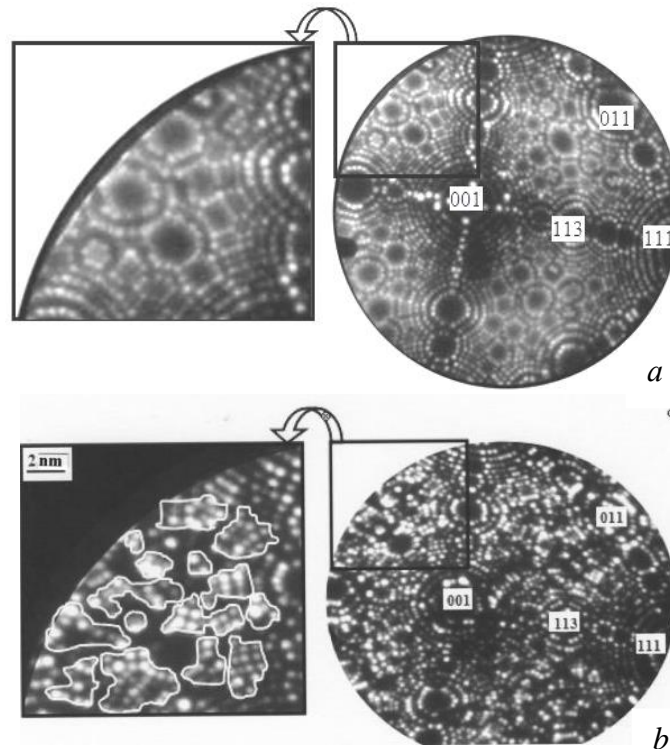


Figure 1. Pt neon images: *a* – ionic contrast of certified crystal; *b* – ionic contrast of surface after irradiation with Ar^+ ions ($F = 10^{16} \text{ ion/cm}^2$).

Figure 2 shows the field ion images of atomic layers of pure Pt irradiated with 30-keV argon ions, depending on their location depth.

As a result of these images computer processing, coordinates of all atoms, their brightness and radii were determined. For describing brightness, a scale of brightness from 0 to 255 units was used. Digital field-ion images transformed to black-and-white patterns were processed.

Figure 3 shows an example of application of the developed software in the analysis of a field-ion image of the first subsurface layer of pure platinum irradiated with a beam of accelerated ions under the above-described conditions.

Figure 4 shows the radii distribution functions $f(R)$ (probability density) for the images of atoms of the 1st, 5th and 81st from surface atomic layers of irradiated platinum. As can be seen, as it approaches the irradiated surface, the distributions width increases significantly. A similar conclusion may be made for the computed brightness distribution functions $f(Y)$ (Figure 5).

It should be noted that the number of imaged atoms in the micropictures increases with distance of the atomic layer from the irradiated surface, varying from 1560 in the 1th layer to 2014 in the 81st layer located at maximum depth in the least damaged zone corresponding to an almost ideal lattice. This correlates to a lower defect ratio of deeper layers (can be assumed that the radius of the tip of emitter remaining practically unvaried in the course of the controlled removal of at least the first dozen atomic layers).

Using the imaged atoms brightness and radii distribution functions, highlighting the zones of the strongest change of field images resulting from ion irradiation may be attempted. Assuming that micropictures of the atomic layers exposed to irradiation include the images of both damaged and undamaged sections of a lattice, and subtracting function $kf_{81}(R)$ with selectable “weight” ($k \leq 1$) from function $f_l(R)$ (where the lower indices denote the layer numbers), we obtain the distribution function for the damaged sections. The latter include images of the atoms with both anomalously low and

anomalously high radii (Figure 6). The sections with anomalously low radii have been formed in a significantly greater number.

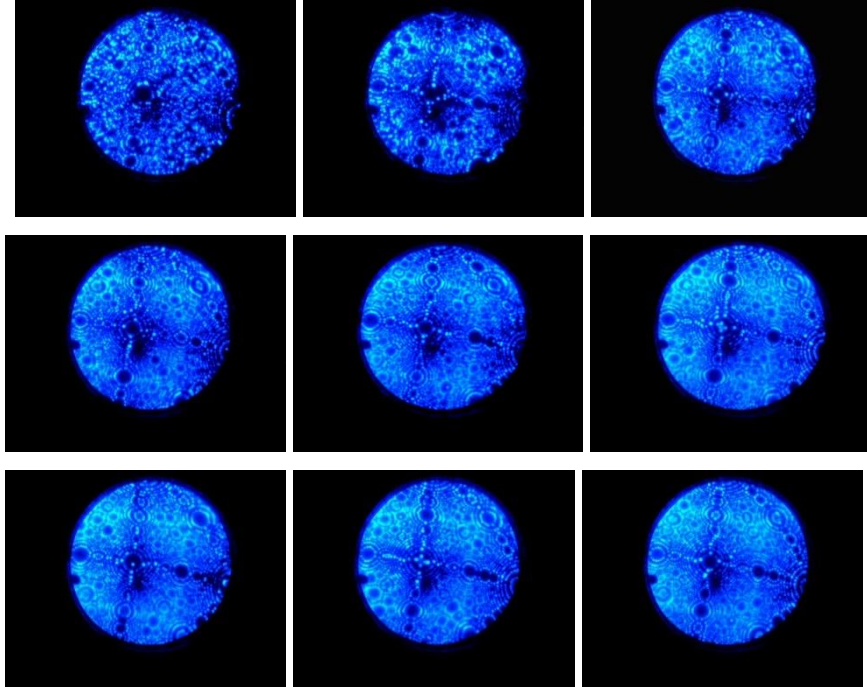


Figure 2. Field ion images of subsurface atomic layers of pure platinum irradiated with Ar^+ ions ($E = 20 \text{ keV}$, $j = 150 \mu\text{A}/\text{cm}^2$, $F = 3.5 \cdot 10^{15} \text{ cm}^{-2}$): 1, 2, 3, 4, 5 – 1st, 2nd, 3rd, 4th and 5th surface atomic layers; 6, 7, 8, 9 – 9th, 10th, 11th and 12th layers (count made by evaporation under field of one atomic layer (001)).

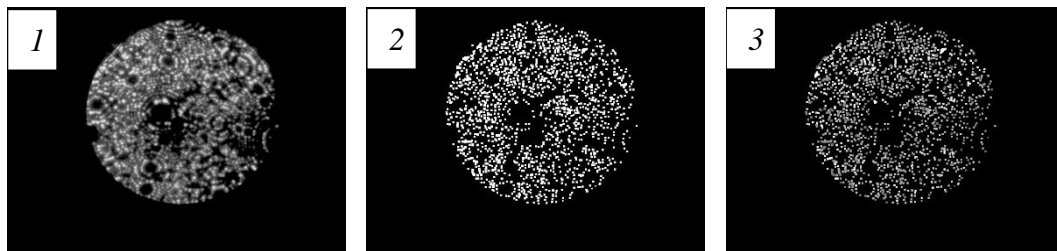


Figure 3. Field ion images of platinum emitter first subsurface layer ($R \sim 30 \text{ nm}$) (a): 1 – experiment; 2 – reconstructed image with defined atomic coordinates (radii and brightness of all imaged atoms are fixed, $R = 2 \text{ ps}$, $Y = 255 \text{ units}$); 3 – synthesized image based on atomic coordinates recognition and computation of atomic brightness and effective radii.

Figure 7 shows the reconstructed image of a picture corresponding to the distribution functions for the 1st and 81st layers (a and b), and to two sections of difference function $f_I(R) - kf_{81}(R)$ (c and d) with anomalously low and anomalously high radii values.

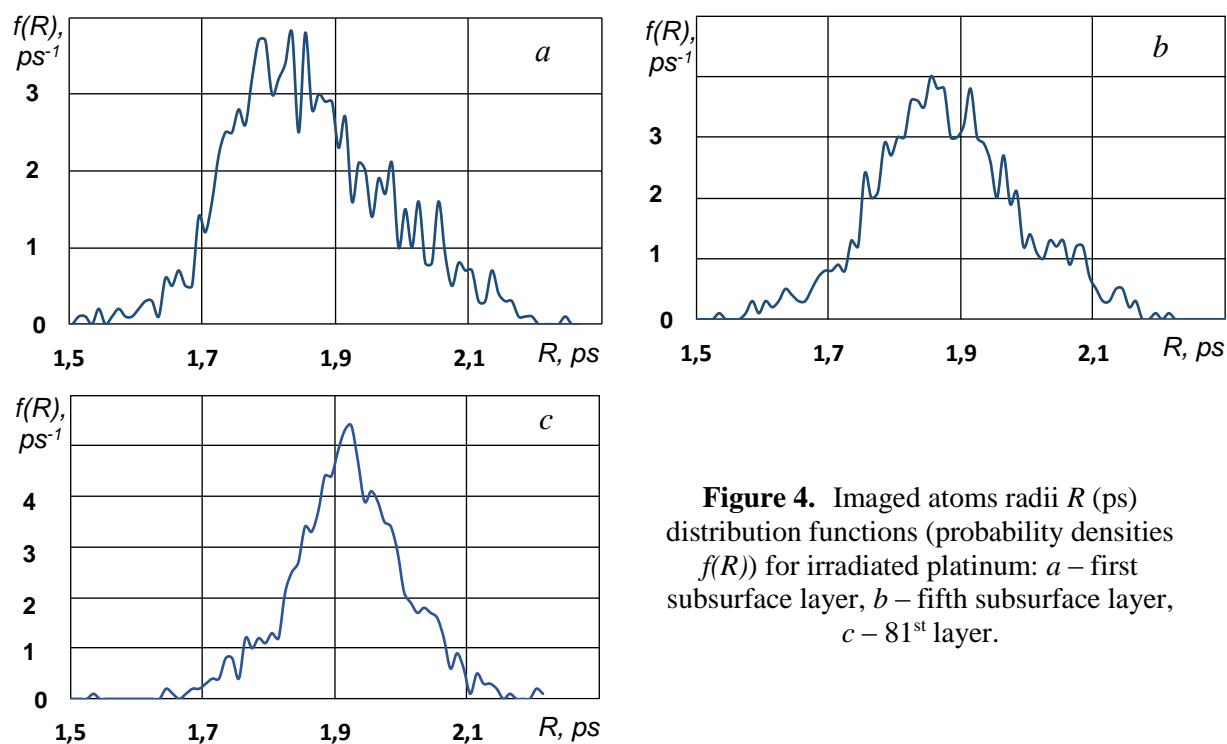


Figure 4. Imaged atoms radii R (ps) distribution functions (probability densities $f(R)$) for irradiated platinum: *a* – first subsurface layer, *b* – fifth subsurface layer, *c* – 81st layer.

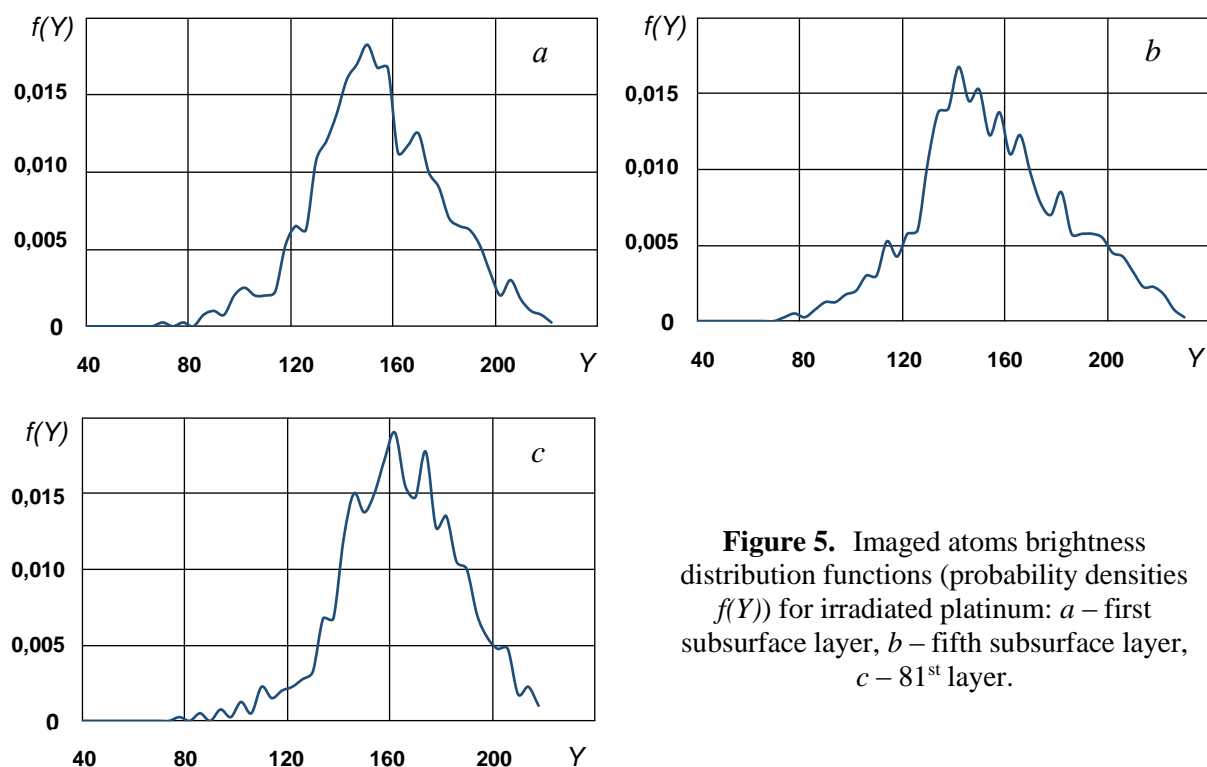


Figure 5. Imaged atoms brightness distribution functions (probability densities $f(Y)$) for irradiated platinum: *a* – first subsurface layer, *b* – fifth subsurface layer, *c* – 81st layer.

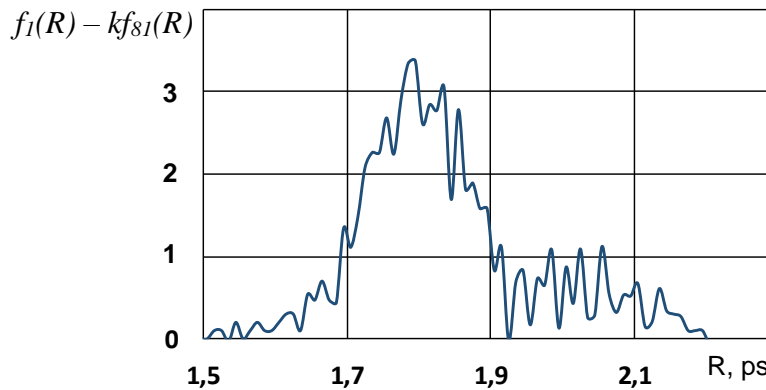


Figure 6. Difference curve $f_1(R) - kf_{81}(R)$ characterizing modified areas of field ion image obtained from the irradiated platinum first subsurface layer ($k = 0.43$).

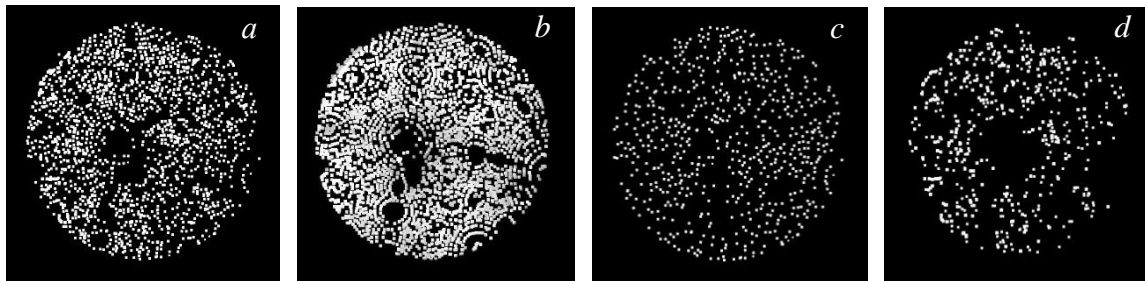


Figure 7. Synthesized field ion images: 1st, 81st atomic layers (*a*, *b*); areas with low (*c*) and high (*d*) radii values in first layer ($Y = 255$).

4. Conclusion

Thus, in the present work we have tested the software for analysis of field ion images of an atomic-pure surface aimed at studying the nature of the effect of Ar^+ ($E = 30$ keV) ions on the atomic structure of subsurface atomic layers in pure platinum (99.99 Pt). The distribution functions for brightness and effective radii values of the imaged atoms have been derived.

As further research, the reconstruction of a 3D picture of defect layers of irradiated platinum (as well as other metals, e.g., W) at arbitrary emitter sections is proposed, potentially displaying several tens of atoms, based on software-derived numerical arrays of such atoms coordinates.

References

- [1] Boowkett K M and Smith D A 1970 *Field Ion Microscopy Defects in Crystalline Solids* (Amsterdam, London: North Holland Publishing Company)
- [2] Muller E W and Tsong T T 1973 *Field ion microscopy, Field ionization and Field evaporation* (Oxford: Pergamon press)
- [3] Kirsanov V V Suvorov A L and Trushin Yu V 1985 *Processes of radiation defect formation in metals* (Moscow: Energoatomizdat)

Acknowledgments

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